# Comment on "A quantum-classical bracket that satisfies the Jacobi identity" [J. Chem. Phys. 124, 201104 (2006)]


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The quantum mechanical description of microscopic systems is nowadays well established and cleanly formulated (at least above the very small Planck scale, where quantum gravity awaits a firmer foundation). However, in many cases, even if the wave equations to be solved are known, they are not easily amenable to a full quantum computation, in practice. A standard approach is then to resort to approximate descriptions of the semiclassical type, where some of the degrees of freedom of the full system are treated quantum mechanically while others are treated at a classical level. In this approach one ends up with a mixed quantum-classical system.

The canonical structures of both classical and quantum mechanics are based on the existence of a Lie bracket between observables, $(A,B)$; this is the commutator in the quantum case and the Poisson bracket in the classical case. The dynamical bracket is such that if $G$ is the infinitesimal generator a symmetry transformation, the variation of an observable $A$ takes the following form

$$\delta A = (A,G)\,\delta\lambda\,. \tag{1}$$

The Lie bracket properties

$$\begin{aligned}
&(aA+bB,C) = a(A,C)+b(B,C) \quad \text{(linearity)},\\
&(A,B) = -(B,A) \quad \text{(antisymmetry)},\\
&((A,B),C)+((B,C),A)+((C,A),B) = 0 \quad \text{(Jacobi)},
\end{aligned} \tag{2}$$

encapsulate the group structure of symmetry transformations, including the dynamical evolution,

$$\frac{d}{dt}A = (A,H) + \frac{\partial}{\partial t}A \tag{3}$$

($H$ being the Hamiltonian), and are therefore crucial for a fully consistent physical description of the classical or quantum system.

In view of this similarity between the classical and quantum formulations, many authors have considered the possibility of finding a consistent description for the abovementioned mixed quantum-classical systems, i.e., systems composed of two interacting sectors, a quantum one and a classical one. Note that such mixed systems are perfectly legitimate as *approximations* to an exact quantum-quantum system, the challenge is, however, to find an *autonomous* and closed description for the mixed case, rather than an intrinsically approximated one. As is well known, ad hoc approximations tend to break exact properties (e.g., symmetries, conservations laws, unitarity, etc) of a theory, while internally consistent approximations tend to preserve them, and so they are, in principle, preferable. (Classical mechanics is precisely an example of a consistent approximation, namely, to quantum mechanics.)

A simple case, often considered in the literature, is that of a one dimensional system with two structureless particles, where $x$ and $k$ are the position and momentum variables of the classical particle, respectively, and $q$ and $p$ those of the quantum particle. $x$ and $k$ commute with everything while $[q,p]=i\hbar$. In this case, the observables are constructed with $x$, $k$, $q$ and $p$,

$$A = \sum_{n,m,r,t} a_{nmrt}\, x^n k^m q^r p^t\,. \tag{4}$$

Minimal requirements for a consistent quantum-classical formulation would include the following:

(i) Symmetry transformations are carried out by a dynamical bracket between observables that must be a Lie bracket.

(ii) The dynamical bracket between two purely quantum observables should reduce to the standard one,

$$(Q,Q') = \frac{1}{i\hbar}[Q,Q'] = \frac{1}{i\hbar}(QQ'-Q'Q)\,, \tag{5}$$

and likewise, for two purely classical observables

$$(C,C') = \{C,C'\} = \frac{\partial C}{\partial x}\frac{\partial C'}{\partial k} - \frac{\partial C}{\partial k}\frac{\partial C'}{\partial x}\,. \tag{6}$$

A standard proposal, made independently by several authors [1, 2], is as follows,

$$(A,B) = \frac{1}{i\hbar}[A,B] + \frac{1}{2}(\{A,B\}-\{B,A\})\,. \tag{7}$$

Unfortunately, this definition fails to satisfy the Jacobi identity. An explicit counterexample is provided in [3], for $A=xq$, $B=xqp$, and $C=k^2p$, since

$$((A,B),C)+((B,C),A)+((C,A),B) = \frac{1}{2}\hbar^2\,. \tag{8}$$

(Jacobi identity violations always come from finiteness of $\hbar$, since in the classical limit any bracket must revert to the Poisson bracket which does satisfy Jacobi.)

In a recent work [4], a new proposal is made, claiming to define a true Lie bracket. No mathematical proof is provided, but it is shown (correctly) that Jacobi is satisfied for the three observables of the example just discussed. Regrettably, as I show below, the Jacobi identity is not satisfied by this new bracket either, if one takes three generic observables.

In the new proposal of [4]

$$(A,B) = (A,B)_q + (A,B)_c \,, \tag{9}$$

with

$$(A,B)_q = \frac{1}{i\hbar}[A,B] \,, \tag{10}$$

as in (7). However, the classical part differs from (7). The new prescription is to take the Poisson bracket of the classical variables involved, while the quantum variables are ordered by moving (commuting) the $q$'s to the left of the $p$'s and setting the $\hbar$ so generated to zero. Of course, this is equivalent to a "normal order" prescription in which $q$ is set to the left of $p$ by hand, $:pq: = qp$. (For simplicity, I use the standard notation $:\quad:$ to denote this "normal order" of operators.) That is,[1]

$$(A,B)_c = \,:\{A,B\}: \,, \tag{11}$$

where the Poisson bracket affects the classical variables. More explicitly, for two observables,

$$\begin{aligned} A &= \sum_{n,m} a_{nm}(x,k)\, q^n p^m \,, \\ B &= \sum_{r,t} b_{rt}(x,k)\, q^r p^t \,, \end{aligned} \tag{12}$$

$a_{nm}(x,k)$ and $b_{rt}(x,k)$ being ordinary functions on the phase space of the classical particle,

$$(A,B)_c = \sum_{n,m}\sum_{r,t} \left\{a_{nm}(x,k), b_{rt}(x,k)\right\} q^{n+r} p^{m+t} \,. \tag{13}$$

As I said, this definition does not preserve the Jacobi identity. An explicit counterexample is provided by the new triple $A = kp$, $B = xp$, and $C = q^2$. For these observables, one easily finds

$$\begin{aligned} (A,B) &= -p^2 \,, \quad ((A,B),C) = 4qp - 2i\hbar, \\ (B,C) &= -2xq \,, \quad ((B,C),A) = -2xk - 2qp, \\ (C,A) &= 2kq \,, \quad ((C,A),B) = 2xk - 2qp, \end{aligned}$$

and hence,

$$((A,B),C) + ((B,C),A) + ((C,A),B) = -2i\hbar \,.$$

Therefore the Jacobi identity is violated. (However, Jacobi is preserved by this triple with the original bracket (7). The same is true whenever the observables involved are at most quadratic in the dynamical variables $x$, $k$, $q$, and $p$, [3].)

Such violation of the Lie bracket property is not surprising; in [3] a no-go theorem was proven (see also [5, 6]), namely, if one requires the quantum-classical bracket to fulfill the rather natural axioms

$$(CQ, C') = \{C, C'\}Q \,, \quad (CQ, Q') = \frac{1}{i\hbar}[Q, Q']C \,, \tag{14}$$

($C$, and $C'$ being purely classical and $Q$ and $Q'$ purely quantum observables), then Jacobi cannot be satisfied. (Note that the bracket (9), with (10) and (13), satisfies the axioms.)

Finally, let me note that in addition to the requirements (i) and (ii), another natural property (common to classical and quantum mechanics) is that the product of two observables $AB$ at $t = 0$ should evolve into the product $A(t)B(t)$ and time $t$ (and similarly for other symmetry transformations). This implies the

(iii) Leibniz rule property for the dynamical bracket,

$$(AB, C) = (A,C)B + A(B,C) \,. \tag{15}$$

As shown in [7], a bracket fulfilling (i-iii) is necessarily either the Poisson bracket (no quantum sector) or the quantum commutator (no classical sector). No quantum-classical mixture is allowed.

In summary, the proposal in [4] does not actually define a Lie bracket since it fails to satisfy the Jacobi identity. Furthermore, any quantum-classical bracket must have awkward properties, as it has to violate rather natural requirements, satisfied both in the purely classical or purely quantum cases. This just means that the quantum-classical mixing remains as a useful but intrinsically approximated approach.

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[1] More precisely,

$$(:\mathcal{A}(x,k,q,p):, :\mathcal{B}(x,k,q,p):)_c =: \{\mathcal{A}(x,k,q,p), \mathcal{B}(x,k,q,p)\}: \,.$$

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